Line Shape of the Pd $M_{45}VV$ Auger Spectrum Determined by Auger-Photoelectron Coincidence Spectroscopy (APECS)

M.T. Butterfield and R.A. Bartynski (Rutgers U.) and S.L. Hulbert (NSLS, Brookhaven National Laboratory)

Abstract No. Butt1099
Beamline: **U16B**

Core valence valence (CVV) Auger spectra contain information about the valence band electronic structure of a solid at the site of the core hole. This technique has been widely used to characterize the local density of states at both impurity and host sites in transition metal alloys. Recently, it has been applied to the class of systems known as surface alloys, where intermixing of the components only occurs in the first atomic layer. A particularly interesting case, which is described in the adjoining report, is the Pd/Ag(100) surface alloy where at low concentrations an anomalous line shape for the Pd $M_{45}VV$ Auger transition is observed [1]. However, in order to better understand that system, we must first determine the intrinsic line shape of the strongly overlapping M_5VV and M_4VV transitions in Pd, so that the modifications of this line shape that occur in the alloy system can be fully understood.

To this end, we have measured the M_5VV and M_4VV Auger spectra in coincidence with Pd $3d_{5/2}$ and $3d_{3/2}$ core photoelectrons, respectively, from a thick Pd film grown on the Ru(0001) surface. Previous studies in our lab have determined that the Pd overlayer grows in an epitaxial Pd(111) structure on this surface, so the spectra should be representative of bulk Pd.

The four coincidence Auger and coincidence photoemission spectra obtained from the Pd film are shown in the Figure below. The M_5VV spectrum gives the intrinsic line shape of the Auger transition since only Pd $3d_{5/2}$ photoelectrons occur at the coincidence energy. Note that considerable intensity from this line lies under the M_4VV line and could not otherwise be observed. The M_4VV coincidence spectrum retains a contribution from the M_5VV line. This is because an appreciable number of inelastically scattered Pd $3d_{5/2}$ photoelectrons have the same kinetic energy as the primary Pd $3d_{3/2}$ line. However, as we have also obtained the coincidence core level spectra, we have enough information to assess the amplitude of this undesired contribution and remove it from the spectrum. Even in the raw coincidence spectra, however, it is clear that the high kinetic energy edge of the M_4VV line differs from that of the M_5VV transition. This is a direct indication that these transitions cannot be described by a simple self-convolution of the valence band density of states (SCDOS), even with a Cini-Sawatzky distortion to account for electron correlation effects. Rather, as we found for the equivalent transitions of Ag, a full description of these lines will require consideration of the multiplet structure of the Pd d^7 configuration. Calculations to evaluate these lines in terms of this multiplet structure are currently underway.

Acknowledgments: This work was supported by the NSF under grants NSF-DMR98-01681 and NSF-DMR-98-12628, by the Petroleum Research Fund under grant ACS-PRF-33750-AC6,5, and the Division of Material Sciences U. S. Department of Energy under Contract No. DE-AC02-98CH10886.

References: [1] P. Weightman and P.T. Andrews, J. Phys. C **12**, L821 (1980).